

Developing an Intelligent Geometric Modelling Framework for the Optimization in the Process of Additive Manufacturing

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Abstract

The focus of this research is the creation of intelligent geometric design technologies. The system employs state-of-the-art methods and tools to automate the arrangement and enhance the placement of 3D shapes. Specifically, the aim is to resolve practical issues in optimizing additive manufacturing processes. This is accomplished by merging artificial intelligence techniques with novel computational solutions for superior results. The article presents a nonlinear optimization approach for solving 3D irregular packing problems with arbitrarily moved and rotated objects. Phi-functions and quasi-Phi-functions are used to describe interactions between the 3D objects. The following formulation presents the packing problem in mathematical terms, along with an analysis of its features. A local optimization algorithm is introduced to identify solutions, with a focus on the characteristics that have been delineated. The results of computational experiments suggest that the proposed solution method is effective for 3D irregular packing optimization.

Keywords

Intelligent system, additive manufacturing, phi-function, mathematical modelling, 3D irregular packing problem, local optimization, non-linear optimization

1. Introduction

This paper proposes the development of intelligent geometric design technologies that leverage advanced methodologies and tools to automate and optimize the placement of geometric objects in space. These technologies address applied challenges in optimizing additive manufacturing by integrating artificial intelligence (AI) and innovative computational approaches to achieve optimal solutions.

Three-dimensional packing problems are a useful model for studying well-established optimization scenarios frequently encountered in various engineering disciplines. There is considerable current momentum towards discovering efficient strategies for tackling these problems. These problems find relevance across various real-world scenarios, including the efficient placement of geometric objects, defined by their shape, within constrained spaces. Frequently, the resolution of a 3D packing challenge entails determining the placement of all provided objects within containers of minimal size.

Packing dilemmas constitute essential elements of mathematical and computational modelling. These problems are inherently challenging due to their intricate interplay with optimization, geometric configuration, and space utilization. These challenges catalyze innovation in the field, particularly in algorithms and computational methodologies. These innovations are vital for

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providing solutions to sophisticated real-world problems in the domains of engineering and science. The advancement and refinement of methodologies for addressing these problems are paramount to the continuous development of natural and information-based systems.

Packing problems are prevalent across many scientific and engineering fields. Often, real-world tests are substituted with computer-based modelling, which greatly minimizes time, physical materials, and overall expenses. Take, for instance, reference [1]; this work explores the most effective ways of arranging objects, which can be turned any which way inside a space that has limits. This study highlights noteworthy enhancements in the effectiveness of packing and the smart use of available resources. Progress in the field has been accelerated by improvements in information technology, specifically when studying particles that vary in size (as is seen in [2]). Reference [3] presents a technique that relies on reinforcement learning; it's used to pack odd 3D shapes into a storage area. This method considers physics and the turning of the shapes to assist. A key feature of this technique is lessening the requirements for learning via the creation of likely moves that aid in training. To elaborate, [4] presents a solver based on learning, focusing on packing objects of any shape.

Applications are numerous and span various domains, including biology, geology, medicine, nanotechnology, robotics, and pattern recognition. These implementations also benefit control systems, vehicle construction, chemistry, power and mechanical engineering, and shipbuilding.

The inherent complexity of packing problems, classified as NP-complete, has spurred the exploration of approximation methods. These methods frequently exhibit a heuristic character. The repertoire includes sophisticated search rules [3,4], the principles of genetic algorithms [5], algorithms inspired by ant and bee behaviors, and simulated annealing [6]. Mathematical programming methods [7,8] and their hybrid or integrated variants [9] constitute further solution approaches.

According to reference [4], the progression of a standard solution algorithm is typically characterized by three repeating phases. The initial phase involves the selection of an order for the objects. The subsequent phase entails the positioning of the objects based on the selected order. The final phase concerns the computation of the objective function's value. It should be noted, however, that the positioning of these objects is subject to several variations, primarily distinguished by the following elements: the trajectory the objects take, the rotation constraints applied, and whether the process tolerates or actively prevents overlap.

Many publications impose restrictions on the rotation of three-dimensional objects, limiting them to specific angles, such as 45 or 90 degrees, or completely prohibiting alterations to an object's orientation. For instance, reference [11] utilizes elementary translational movement to arrange convex polytopes. Lamas-Fernandez et al. (2023) have also developed voxel-based approaches to address the 3D irregular packing problem [13]. The research in [12] introduces the HAPE3D algorithm, which focuses on packing polyhedra with rotations limited to eight predetermined angles around the coordinate axes. Finally, the study documented in [14] concludes that determining object orientations across a full 360-degree range in 3D is not a practical solution.

In the face of the daunting task of developing meaningful mathematical models, formulating equivalent expressions for continuous rotations of three-dimensional geometric figures is a pursuit by a select few researchers. In this context, techniques for ellipsoid packing are examined, leveraging both continuous and differentiable nonlinear optimization strategies, as demonstrated in [15, 16]. Packaging multiple convex 3D objects is the primary subject of discussion in reference [17].

This research is devoted to developing an intelligent system that will optimize the 3D printing process of many industrial parts using unique intellectual tools and technologies for modelling and solving optimization problems of geometric design. The proposed approach involves modelling and solving the optimization problem of packing non-convex geometric objects.

To this end, a multifaceted approach is employed, integrating mathematical and computer simulation methodologies. These methodologies are meticulously designed to accurately capture the interactions (non-intersection conditions) between geometric objects. This strategy enables formulating the primary problem as a nonlinear optimization problem. The mathematical underpinnings of our methodology are rooted in the phi-functions method, exhaustively delineated in [17]. This method provides a rigorous analytical representation of both the constraints that prevent intersection and the constraints that ensure the location of objects in the container. A critical aspect of our methodology is the incorporation of continuous rotational transformations

and parallel translational motions of objects, ensuring a comprehensive and precise representation of the geometric constraints.

The primary goal of this research is to develop an intelligent geometric design system that enhances the automation and optimization of 3d shape arrangement, particularly for additive manufacturing (3d printing) applications. The work seeks to improve packing efficiency by integrating artificial intelligence (AI) with advanced computational geometry techniques.

This research advances the field of intelligent geometric design by introducing a novel optimization framework for 3d irregular packing. Combining AI techniques with computational geometry provides a viable additive manufacturing solution, demonstrating theoretical innovation and industrial applicability. The computational experiments confirm the method's effectiveness, paving the way for smarter, more efficient manufacturing processes.

2. Problem definition

The proposed intellectual system is predicated on a distinctive universal mathematical model of optimization geometric design, constructed with specialized intellectual means of modelling this category of problems. These intellectual means encompass specific functions designated as "phi-functions" [18]. These functions facilitate the construction of a generalized universal mathematical model in the form of a nonlinear optimization problem.

Let there be the following convex geometric objects:

- a convex polyhedron J_1 given by vertices $p_{1t} = (p_{1t}^1, p_{1t}^2, p_{1t}^3), t \in T_1 = \{1, 2, \dots, Q_1\};$
- a circular cylinder $J_2 = \{X \in \mathbb{R}^3, x^2 + y^2 - R_2^2 \leq 0, 0 \leq z \leq H_2\};$
- a sphere $J_3 = \{X \in \mathbb{R}^3, x^2 + y^2 + z^2 - R_3^2 \leq 0\};$
- a circular cone $J_4 = \{X \in \mathbb{R}^3, x^2 + y^2 - c_4^2(z - E_4)^2 \leq 0, z \geq 0, E_4 > 0\};$
- a truncated circular cone $J_5 = \{X \in \mathbb{R}^3, x^2 + y^2 - c_5^2(z - E_5)^2 \leq 0, E_5 \geq H_5 \geq 0, 0 \leq z \leq H_5\};$
- a spherical segment $J_6 = \{X \in \mathbb{R}^3, x^2 + y^2 + (z + H_6)^2 - R_6^2 \leq 0, z - H_6 \leq 0, 0 < H_6 < R_6\};$
- a half-space $J_7 = \{X \in \mathbb{R}^3, z \leq 0\}.$

We suppose that each concave geometric objects $Q_i, i \in I = \{1, 2, \dots, n\}$, is a finite union of convex geometric objects $O_i = \sum_{k=1}^{\kappa_i} O_{ik}$ where O_{ik} are geometric objects of kind $J_r, r = 1, 2, \dots, 7$.

The location of each object O_{ik} with respect to the local coordinate system of O_i is given with placement parameters $u_{ik} = (v_{ik}, \theta_{ik}), k \in K_i = \{1, 2, \dots, \kappa_i\}$.

A container C can be a rectangular parallelepiped (rectangular prism or cuboid) $\mathbb{C}_1 = \{X \in \mathbb{R}^3, w_1 \leq x \leq w_2, l_1 \leq y \leq l_2, \eta_1 \leq z \leq \eta_2\}$, where $w_1 \geq 0, l_1 \geq 0, \eta_1 \geq 0$, or a right circular cylinder \mathbb{C}_2 with height $h = h_2 - h_1$ ($h_2 \geq h_1$) and radius r , or a solid sphere $\mathbb{C}_3 = \{X \in \mathbb{R}^3, x^2 + y^2 + z^2 - R^2 \leq 0\}.$

Basic problem. Pack geometric objects $O_j, i \in I$, without their mutual overlapping in the container C so that its volume will reach the minimum value.

We assume

$$\tilde{r} = \begin{cases} (w_1, w_2, l_1, l_2, \eta_1, \eta_2) \in \mathbb{R}^6 \text{ if } \mathbb{C} = \mathbb{C}_1, \\ (r, h) \in \mathbb{R}^2 \text{ if } \mathbb{C} = \mathbb{C}_2, \\ r \in \mathbb{R}^1 \text{ if } \mathbb{C} = \mathbb{C}_3. \end{cases}$$

Geometric objects O_i (in what follows objects) both are allowed to be translated by a vector $v_i = (x_i, y_i, z_i)$ and to rotate by angles $\theta_i = (\varphi_i, \psi_i, \omega_i)$. Hence, a vector $u_i = (v_i, \theta_i) = (x_i, y_i, z_i, \varphi_i, \psi_i, \omega_i)$ gives a location of O_i in \mathbb{R}^3 . Thus, the vector $u = (u_1, u_2, \dots, u_n) \in \mathbb{R}^{6n}$ gives the location of all $O_i, i \in I$, in \mathbb{R}^3 .

Then, components of the vector $(u, \mathcal{R}) = (u_1, u_2, \dots, u_n, \mathcal{R}) \in \mathbb{R}^{6n+m}$, where m can be either 1 or 3 or 6, form a complete set of variables. In addition, an object O_i translated by a vector v_i and rotated through angles θ_i is designated by $O_i(u_i)$ and a container \mathbb{C} with variable size \mathcal{R} is denoted as $\mathbb{C}(\mathcal{R})$.

3. Mathematical model

On the ground of phi-functions [17,18] and quasi-phi-functions [19,20], a mathematical formulation of the problem can be stated as follows:

$$(u^{\mathcal{C}}, \mathcal{R}^{\mathcal{C}}, Z^{\mathcal{C}}) = \operatorname{argmin} H(\mathcal{R}) \text{ s.t. } (u, \mathcal{R}, Z) \in \Lambda \subset \mathbb{R}^N \quad (1)$$

$$\Lambda = \{(u, \mathcal{R}, Z) \in \mathbb{R}^N : \Phi_{ij}(u_i, u_j, \mathbb{Z}_{ij}) \geq 0, i < j \in I, \\ \Phi_i(u_i, \mathcal{R}) \geq 0, i \in I, L(\mathcal{R}) \geq 0\} \quad (2)$$

where

$$H(\mathcal{R}) = \begin{cases} (w_2 - w_1)(l_2 - l_1)(\eta_2 - \eta_1) & \text{if } \mathbb{C} = \mathbb{C}_1, \\ (h_2 - h_1)r^2 & \text{if } \mathbb{C} = \mathbb{C}_2, \\ r^3 & \text{if } \mathbb{C} = \mathbb{C}_3, \end{cases}$$

$$L(\mathcal{R}) = \begin{cases} w_1 \geq 0, l_1 \geq 0, \eta_1 \geq 0, w_2 - w_1 \geq 0, l_2 - l_1 \geq 0, \eta_2 - \eta_1 \geq 0 & \text{if } \mathbb{C} = \mathbb{C}_1, \\ h_2 - h_1 \geq 0, h_1 \geq 0, r \geq 0 & \text{if } \mathbb{C} = \mathbb{C}_2, \\ r \geq 0 & \text{if } \mathbb{C} = \mathbb{C}_3, \end{cases}$$

$$N \geq 6n + m, m = \begin{cases} 6 & \text{if } \mathbb{C} = \mathbb{C}_1, \\ 3 & \text{if } \mathbb{C} = \mathbb{C}_2, \\ 1 & \text{if } \mathbb{C} = \mathbb{C}_3. \end{cases}$$

Here, the inequality $\Phi_{ij}(u_i, u_j, \mathbb{Z}_{ij}) \geq 0$ ensures non-overlapping O_i and O_j while the inequality $\Phi_i(u_i, \mathcal{R}) \geq 0$ guarantees a containment of O_i within $\mathbb{C}(\mathcal{R})$ i.e. $\Phi_i(u_i, \mathcal{R})$ is a *phi*-function for O_i and $B(\mathcal{R}) = \mathbb{R}^3 \setminus \operatorname{int} \mathbb{C}(\mathcal{R})$ where $\operatorname{int} \mathbb{C}(\mathcal{R})$ is the interior of \mathbb{C} . A vector \mathbb{Z}_{ij} can consist of at most q components.

Let us examine the fundamental properties of the mathematical model.

Since $O_i = \bigcup_{s=1}^{\epsilon_i} O_{is}$ and $O_j = \bigcup_{p=1}^{\epsilon_j} O_{jp}$, then $O_i \cap O_j = \emptyset$ if $O_{is} \cap O_{jp} = \emptyset$, $s \in K_i$, $p \in K_j$. Consequently $\Phi_{ij}(u_i, u_j, \mathbb{Z}_{ij}) = \min\{\Phi_{ij}^{sp}(u_i, u_j, \mathbb{Z}_{ij}^{sp}), s \in K_i, p \in K_j\}$ where $\Phi_{ij}^{sp}(u_i, u_j, \mathbb{Z}_{ij}^{sp})$ is either a Φ -function or a quasi-phi-function for O_{is} and O_{jp} . Thus, $\Phi_{ij}(u_i, u_j, \mathbb{Z}_{ij}) \geq 0$ if $\min\{\Phi_{ij}^{sp}(u_i, u_j, \mathbb{Z}_{ij}^{sp}), s \in K_i, p \in K_j\} \geq 0$.

Each quasi Φ -function $\Phi_{ij}^{sp}(u_i, u_j, \mathbb{Z}_{ij}^{sp})$ in general, is a function of the kind $\Phi_{ij}^{sp}(u_i, u_j, \mathbb{Z}_{ij}^{sp}) = \max\{\Psi_{ij}^{spa}(u_i, u_j, \mathbb{Z}_{ij}^{sp}), a \in A_{ij}^{sp} = B_{ij}^{sp} \cup \mathbb{C}_{ij}^{sp} = \{1, 2, \dots, a_{ij}^{sp} + 1, a_{ij}^{sp} + 2, \dots, \kappa_{ij}^{sp}\}\}$. Thus, $\Phi_{ij}^{sp}(u_i, u_j, \mathbb{Z}_{ij}^{sp}) \geq 0$ if no fewer than one of the inequality systems $\{\Psi_{ij}^{spa}(u_i, u_j, \mathbb{Z}_{ij}^{sp}) \geq 0, a \in A_{ij}^{sp}\}$, holds true. It is evident $\Phi_{ij}(u_i, u_j, \mathbb{Z}_{ij}) \geq 0$ if at least one of the inequality systems $\{\Psi_{ij}^{spa}(u_i, u_j, \mathbb{Z}_{ij}^{sp}) \geq 0, s \in K_i, p \in K_j\}$, where $a \in A_{ij}^{sp}$ is satisfied. So, the number of systems is $\varsigma_{ij} = \prod_{s=1}^{\kappa_i} \prod_{p=1}^{\kappa_j} \kappa_{ij}^{sp}$. For the sake of convenience, we rename the inequality systems as

$$\{\Psi_{ij}^t(u_i, u_j, \mathbb{Z}_{ij}^t) \geq 0, t \in T_{ij} = \{1, 2, \dots, \varsigma_{ij}\}.$$

It follows from the previous items that $\Phi_{ij}(u_i, u_j, \mathbb{Z}_{ij}) \geq 0, i < j \in I$, if at least one of the inequality systems $\{\Psi_{ij}^t(u_i, u_j, \mathbb{Z}_{ij}^t) \geq 0, i < j \in I, \text{ where } t \in T_{ij}, \text{ holds true. For the sake of convenience, we rename the inequality systems as}$

$$G_\tau(u, \mathbb{Z}) \geq 0, \tau \in Y = \{1, 2, \dots, \vartheta\}$$

$$\text{where } \vartheta = \prod_{i=1}^n \prod_{j=1}^n \varsigma_{ij}.$$

Each function of the family $\Psi_{ij}^{spa}(u_i, u_j, \mathbb{Z}_{ij}^{sp}), a \in \mathbb{C}_{ij}^{sp}$ contains an additional vector \mathbb{Z}_{ij}^{sp} consisting in general of several components. This means that each inequality system contains at most $\prod_{i=1}^{\kappa_i} \prod_{j=1}^{\kappa_i} \kappa_i \kappa_j$ variables.

Each function $\Phi_i(u_i, \mathcal{H})$ is presented as

$$\Phi_i(u_i, \mathcal{H}) = \min \{ \Phi_{is}(u_i, \mathcal{H}), s \in K_i = \{1, 2, \dots, \kappa_i\} \}$$

where $\Phi_{is}(u_i, \mathcal{H})$ is the Φ -function for O_{is} and $C(\mathcal{H}) = R^3 \setminus \text{int } \mathbb{C}(\mathcal{H})$.

Based on items 3 and 4 we draw a very important conclusion: the feasible region Λ can be presented as follows:

$$\Lambda = \bigcup_{\tau=1}^{\vartheta} \Lambda_\tau,$$

where Λ_τ is specified by the inequality system

$$F_\tau(u, \mathcal{H}, \mathbb{Z}_\tau) = \begin{cases} G_\tau(u, \mathbb{Z}_\tau) \geq 0, \\ \Phi_i(u_i, \mathcal{H}) \geq 0, i \in I, \\ L(\mathcal{H}) \geq 0, \end{cases} = \begin{cases} f_{\tau 1}(\xi_{\tau 1}) \geq 0, \\ f_{\tau 2}(\xi_{\tau 2}) \geq 0, \\ \dots\dots\dots \\ f_{\tau \epsilon}(\xi_{\tau \epsilon}) \geq 0 \end{cases}$$

where $\xi_{\tau \epsilon}$ consists of components of vectors u and \mathbb{Z}_τ , $\epsilon > \prod_{i=1}^{\kappa_i} \prod_{j=1}^{\kappa_i} \kappa_i \kappa_j + n \prod_{i=1}^n \kappa_i$.

Note that the functions $f_{\tau j}(\xi_{\tau j}), j = 1, 2, \dots, \epsilon$, are smooth with respect to their variables.

Consequently, solving the problem (1) – (2) can be reduced to solving step by step the following subproblems:

$$(u^{\tau}, \mathcal{H}^{\tau}) = \text{argmin } H(\mathcal{H}) \text{ s.t. } (u, \mathcal{H}) \in \Lambda_\tau \subset \mathbb{R}^N, \tau \in Y.$$

This means we have a theoretical chance to compute a global minimum solution of the problem (1) – (2).

4. Solution algorithm

Since the solution space of the stated problem is defined by many inequalities, we propose solving the problem (1)–(2) in stages to obtain a local minimum point within a reasonable time.

1. Derivation of starting points from the feasible region.

- First of all, we cover objects O_i by spheres S_i of minimum radii $r_i^0, i \in I$.
- Then we pack in pairs of objects $O_i, i \in I$, into clusters to be either cuboids or spheres of minimum volumes. (If the number n of geometric objects is less than 30, then we cover O_i by spheres S_i of minimum radii $r_i, i \in I$, and pack the spheres into the container \mathbb{C} with minimum volume).
- We solve a packing problem of the clusters into a container C with minimum volume.
- Next, we take appropriate objects $O_i, i \in I$, instead of spheres $S_i, i \in I$, (in addition, we give rotation angles of $O_i, i \in I$, randomly) or clusters $Q_t, t \in T$, and form a starting point belonging to the feasible region.

2. Calculation of a local minimum.

- We solve the packing problem of objects $O_i, i \in I$, with fixed angle parameters, obtain a local minimum point.

- On the ground of the point and given angle parameters, a starting point is formed, and a local minimum point of the problem (1) – (2) is calculated.
Let us consider the stages in detail.

5. Constructing feasible starting points

5.1. Covering geometric objects with spheres

In order to cover objects O_i with spheres $S_i = \{X \in \mathbb{R}^3, x^2 + y^2 + z^2 - r_i^2 \leq 0\}$ of minimum radii r_i , with placement parameters $v_i = (x_i, y_i, z_i), i \in I$, we solve the following problems:

$$r_i^0 = \min r_i \text{ s.t. } (r_i, v_i) \in D_i \subset \mathbb{R}^4, i \in I, \\ D_i = \{(r_i^0, v_i^0) \in \mathbb{R}^4, \Phi_i(r_i, v_i) \geq 0\}.$$

Here, $\Phi_i(r_i, v_i) \geq 0$ provides non-overlapping O_i and a set

$$\mathbb{C}_i = \{X \in \mathbb{R}^3, -(x - x_i)^2 - (y - y_i)^2 - (z - z_i)^2 + r_i^2 \geq 0\}.$$

As a result of solving the problem, a point (r_i^0, v_i^0) is calculated. In what follows, we remove the origins of the incoordinate systems of O_i so that they coincide with the centers of spheres $S_i, i \in I$. This means that a translation vector of O_i in \mathbb{R}^3 is a vector $v_i = (x_i, y_i, z_i)$ which coincides with the centre coordinates of the sphere \mathbb{C}_i .

After that, we solve a packing problem of spheres $S_i, i \in I$, into a sphere \mathbb{C}_3 of minimum volume if $n \leq 30$. The problem is solved just as presented in [18]. Consequently, a point $(v^{\hat{i}}, R^{\hat{i}})$ close to a global minimum point is identified. Randomly given rotation angles $\varphi_i = \varphi_i^0, \psi_i = \psi_i^0$ and $\omega_i = \omega_i^0$ of $O_i, i \in I$, we form a starting point $(u^0, \theta^0) = (v^{\hat{i}}, \varphi^0, \psi^0, \omega^0) \in \Lambda$ for the problem (1) – (2) for $\mathbb{C} = \mathbb{C}_3$.

5.2. Pairwise packing of objects into clusters

Let $O_i, i \in I$, consist of k groups each containing l_k identical geometric objects. We pack in pairs $O_i, i \in I$, into cuboids Q_{ij} of the minimum volumes $V_{ij}^C, i < j \in K = \{1, 2, \dots, k\}$. To this end, we solve the problems

$$V_{ij}^C = F_{ij}(\hat{\mathcal{N}}) = \min F_{ij}(\hat{\mathcal{N}}) \text{ s.t. } (u_i, u_j, \hat{\mathcal{N}}) \in \Omega_{ij} \subset \mathbb{R}^{18}, i < j \in I, \quad (3)$$

where

$$F_{ij}(\hat{\mathcal{N}}) = (w_2^{ij} - w_1^{ij})(l_2^{ij} - l_1^{ij})(\eta_2^{ij} - \eta_1^{ij}), \\ \Omega_{ij} = \{(u_i, u_j, \hat{\mathcal{N}}) \in \mathbb{R}^{18} : \Phi_{ij}(u_i, u_j) \geq 0, \Phi_i(u_i, \hat{\mathcal{N}}) \geq 0, \Phi_j(u_j, \hat{\mathcal{N}}) \geq 0, L_{ij}(\hat{\mathcal{N}}) \geq 0\}, \\ L_{ij}(\hat{\mathcal{N}}) = (w_1^{ij} \geq 0, l_1^{ij} \geq 0, \eta_1^{ij} \geq 0, w_2^{ij} - w_1^{ij} \geq 0, l_2^{ij} - l_1^{ij} \geq 0, \eta_2^{ij} - \eta_1^{ij} \geq 0).$$

The inequality $\Phi_{ij}(u_i, u_j) \geq 0$ insures $\text{int } O_i \cap \text{int } O_j = \emptyset$ while $\Phi_i(u_i, \hat{\mathcal{N}}) \geq 0$ guarantees a placement of O_i within Q_{ij} .

Consequently, a local minimum point $(u_i^{\hat{i}}, u_j^{\hat{i}}, \hat{\mathcal{N}}^{\hat{i}})$ close to a global minimum for the problem (3) is computed.

After that, we pack in pairs $O_i, i \in I$, into spheres S_{ij} of the minimum radius $R_{ij}^{\hat{i}}, i < j \in K = \{1, 2, \dots, k\}$, i.e. we solve the following problems:

$$V^S = \frac{4}{3} \pi \min \{R_{ij}^3, i < j \in I\} \text{ s.t. } (u_i, u_j, R_{ij}) \in \Omega_{ij} \subset \mathbb{R}^{13},$$

where

$$\Omega_{ij} = \{(u_i, u_j, R_{ij}) \in \mathbb{R}^{16} : \Phi_{ij}(u_i, u_j) \geq 0, \Phi_i(u_i, R_{ij}) \geq 0, \Phi_j(u_j, R_{ij}) \geq 0, R_{ij} \geq 0\}.$$

The inequality $\Phi_{ij}(u_i, u_j) \geq 0$ provides $\text{int } O_i \cap \text{int } O_j = \emptyset$ while $\Phi_i(u_i, \hat{\mathcal{N}}) \geq 0$ insures arrangement of O_i within S_{ij} .

Let point (u_i^*, u_j^*, R_{ij}^*) be an approximate point to a global minimum point of the problem.

To derive a starting point belonging to Ω_{ij} , we introduce homothetic coefficients h_i of objects O_i and O_j and assume that the coefficients are variable. Thus, we have the opportunity to enlarge or diminish sizes of objects O_i and O_j changing their homothetic coefficients. Consequently, the Φ -function for $O_i(u_i, h_i)$ and $O_j(u_j, h_j)$ depends on h_i and h_j , i.e. the Φ -function takes the form $\Phi_{ij}(u_i, u_j, h_i, h_j)$, and the Φ -function for $O_i(u_i, h_i)$ and $cl(\mathbb{R}^3 \setminus \mathbb{C}_{ij})$ where \mathbb{C}_{ij} is either Q_{ij} or S_{ij} , depends on h_i , i.e. the Φ -function has the kind $\Phi_i(u_i, \tilde{h}, h_i)$. Since for any $0 < h_i < \infty$, objects $O_i(u_i, h_i)$ are homothetic, then $\Phi_{ij}(u_i, u_j, h_i, h_j)$ and $\Phi_i(u_i, h_i, \tilde{h})$ have the same form for any $0 < h_i < \infty$. The homothetic coefficients $h_i, i \in T$, form a vector $h = (h_i, h_j) \in \mathbb{R}^2$. Furthermore, we select such sizes \tilde{h}' of container $\mathbb{C}_{ij}(\tilde{h}')$ which guarantees placement of objects O_i and O_j into $\mathbb{C}_{ij}(\tilde{h}')$ and fix \tilde{h}' . It permits to formulation the helper problem

$$\sum_{i=1}^g h_i^{\tilde{h}'} = \max \sum_{i=1}^g h_i s. t. (u, h) \in \Delta \subset \mathbb{R}^{14}, \quad (4)$$

where

$$\Delta = \{(u, h) \in \mathbb{R}^{14}, \Phi_{ij}(u_i, u_j, h_i, h_j) \geq 0, \Phi_k(u_k, h_k) \geq 0, h_k \geq 0, h_k - 1 \geq 0, k = i, j\}.$$

A starting point (u_i', u_j', h') for the problem is formed in the following manner. We set $h_k' = 0.01$, $k = i, j$, and randomly assign u' so that $v_k' \in C_{ij}(\tilde{h}')$, $k = i, j$. Note that due to $h_k' = 0.01, k \in i, j$, we generally have the point $(u_i', u_j', h') \in \Delta$.

It is evident if $h_k^{\tilde{h}'} = 1, k = i, j$, then (u_i^*, u_j^*, h^*) is a global maximum point of the problem (4), ensuring objects O_i and O_j are packed into $\mathbb{C}_{ij}(\tilde{h}')$.

Now taking the point (u_i', u_j', h') as a starting one, we tackle the problem (4) and obtain a global maximum point $(u_i^*, u_j^*, 1)$.

6. Local optimization

6.1. Packing geometric objects without rotations

The stage involves packing objects under fixed rotation angles.

Firstly, we fix the values of the rotation angles $\varphi_i = \varphi_i^0, \psi_i = \psi_i^0$ and $\omega_i = \omega_i^0, i \in I$. This means that only translations of objects $O_i, i \in I$ are allowed. In this case, the problem (1) – (2) takes the form

$$H(\tilde{h}^{\tilde{h}'}) = \min H(\tilde{h}) s. t. X \in \Theta \subset \mathbb{R}^D \quad (5)$$

where

$$\Theta = \{X = (v, \tilde{h}, Z) \in \mathbb{R}^D : \Phi_{ij}(v_i, v_j, Z_{ij}) \geq 0, 0 < i < j \in I, \Phi_i(v_i, \tilde{h}) \geq 0, i \in I, L(\tilde{h}) \geq 0\}, D \geq 3n + m.$$

For computing a local minimum point $(v^{0*}, \tilde{h}^{0*}, Z^{0*})$ of the problem, the same solution scheme is applied to solving the problem (1) – (2).

6.2. Searching for a local minimum point of the basic problem

Now we continue to search for a local minimum point $(u^{0*}, \tilde{h}^{0*}, Z^{0*})$ of the problem (1) – (2), beginning with a starting point $(u^0, \tilde{h}^0, Z^0) = (v^{0*}, \theta^0, \tilde{h}^{0*}, Z_{\kappa}^{0*}) \in \Lambda$ where rotation angles θ^0 and $(v^{0*}, \tilde{h}^{0*}, Z_{\kappa}^{0*})$ are taken from a local minimum point of the problem (5). This stage consists of

several steps, which are reduced to solving a sequence of substantially simpler subproblems regarding the number of inequalities and the dimensions of the solution space.

Computing a local minimum point (v^*, \tilde{h}^*, Z^*) of the problem (1) – (2) can be reduced to solving a sequence of subproblems

$$H(\tilde{h}^{(\kappa+1)*}) = \min H(\tilde{h}) \text{ s.t. } X \in \Lambda_\kappa, \kappa=0,1,2,\dots \quad (6)$$

For each starting point $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*) \in \Lambda$ a subregion Λ_κ containing the point $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*)$ is singled out. A starting point is $(u^{0*}, \tilde{h}^{0*}, Z_0^*) = (u^0, \tilde{h}^0, Z_0^0)$. A vector $Z_\kappa^{\dot{\iota}}$ is constructed specially.

The computational process proceeds until $H(\tilde{h}^{(\kappa+1)*}) = H(\tilde{h}^{\kappa*})$ is fulfilled. This indicates that the point $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*)$ is a local minimum point of the problem (1) – (2).

6.3. Transition between feasible subregions

Since $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*)$ being a local minimum point of the problem $H(\tilde{h}^{\kappa*}) = \min H(\tilde{h})$ s.t. $X \in \Lambda_\kappa$ is not in generally a local minimum point of the problem (1) – (2), we need to transition to another region $\Lambda_{\kappa+1}$ which ensures the value of $H(\tilde{h})$ does not worsen at the local minimum point $\dot{\iota}$ in the new region $\Lambda_{\kappa+1}$.

Let $f_{ij\kappa}(\xi_{ij}) \geq 0$, $j \in N_\kappa$, be active inequalities at the point $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*)$. We single out inequality subsystems $\Psi_{ij}^{spa}(u_i, u_j, Z_{ij}^{spa}) \geq 0$, $i \in E_{1\kappa}, j \in E_{2\kappa}, s \in K_{i\kappa}, p \in K_{j\kappa}, a = a_{ij}^{sp}$, where t_{ij}^{sp} is from the index set A_{ij}^{sp} , which contain the active inequalities. Note that $\Psi_{ij}^{spa}(u_i^\kappa, u_j^\kappa, Z_{ij}^{spa}) = 0$, $i \in E_{1\kappa}, j \in E_{2\kappa}, s \in K_{i\kappa}, p \in K_{j\kappa}$.

Next, we single out inequalities $\Phi_{ij}^{sp}(u_i, u_j, Z_{ij}^{sp}) \geq 0$ from the inequality system (2), which incorporates the inequality subsystems $\Psi_{ij}^{spa}(u_i, u_j, Z_{ij}^{spa}) \geq 0$, $i \in E_{1\kappa}^0 \subset E_{1\kappa}, j \in E_{2\kappa}^0 \subset E_{2\kappa}, s \in K_{i\kappa}^0 \subset K_{i\kappa}, p \in K_{j\kappa}^0 \subset K_{j\kappa}, t = t_{ij}^{sp}$. Then, we compute the components Z_{ij}^{spa} , $i \in E_{1\kappa}^0, j \in E_{2\kappa}^0, s \in K_{i\kappa}^0, p \in K_{j\kappa}^0, a \in C_{ij}^{sp}$, as the solution to the problems and select components Z_{ij}^{spt} , $t \in C_{ij\kappa}^{sp} \subset C_{ij}^{sp}$ for which $\Psi_{ij}^{spa}(u_i^\kappa, u_j^\kappa, Z_{ij}^{sa*})_{ij}^{sp*} > 0$.

After that, we compute $\Phi_{ij}^{sp}(u_i^\kappa, u_j^\kappa, Z_{ij}^{spa}) = k_{ij}^{spa}$, $i \in E_{1\kappa}, j \in E_{2\kappa}, s \in K_{i\kappa}, p \in K_{j\kappa}, a \in B_{ij}^{sp} \cup C_{ij\kappa}^{sp}$. Since each of $\Phi_{ij}^{sp}(u_i, u_j, Z_{ij}^{spa})$, $i \in E_{1\kappa}, j \in E_{2\kappa}, s \in K_{i\kappa}, p \in K_{j\kappa}$, includes operation \max then some of k_{ij}^{spt} , $i \in E_{1\kappa}, j \in E_{2\kappa}, s \in K_{i\kappa}, p \in K_{j\kappa}, t \in B_{ij\kappa}^{sp} \cup C_{ij\kappa}^{sp}$ ($B_{ij\kappa}^{sp} \subset B_{ij}^{sp}$) can be found strictly positive. Let $\Phi_{ij}^{sp}(u_i^\kappa, u_j^\kappa, Z_{ij}^{spq}) = \Psi_{ij}^{spq}(u_i^\kappa, u_j^\kappa, Z_{ij}^{spq}) = k_{ij}^{spq} > 0$, $i \in E_{1\kappa}^0 \subset E_{1\kappa}^1, j \in E_{2\kappa}^0 \subset E_{2\kappa}^0, s \in K_{i\kappa}^0 \subset K_{i\kappa}, p \in K_{j\kappa}^0 \subset K_{j\kappa}, q \in B_{ij\kappa}^{sp} \cup C_{ij\kappa}^{sp}$ where $B_{ij\kappa}^{sp} \subset B_{ij}^{sp}$. Since $a \neq q$ for all $i \in E_{1\kappa}^0, j \in E_{2\kappa}^0, s \in K_{i\kappa}^0, p \in K_{j\kappa}^0, a \in B_{ij\kappa}^{sp} \cup C_{ij\kappa}^{sp}$, we can derive a new inequality system $F_{\kappa+1}(u, \tilde{h}, Z_{\kappa+1}) \geq 0$ specifying a new feasible subregion $\Lambda_{\kappa+1}$ by substituting the inequality subsystems $\Psi_{ij}^{spa}(u_i, u_j, Z_{ij}^{spa}) \geq 0$, $i \in E_{1\kappa}^0, j \in E_{2\kappa}^0, s \in K_{i\kappa}^0, p \in K_{j\kappa}^0, t = t_{ij}^{sp}$, in the system $F_\kappa(u, \tilde{h}, Z_\kappa) \geq 0$ for the inequality subsystems $\Psi_{ij}^{spq}(u_i, u_j, Z_{ij}^{spq}) \geq 0$, $i \in E_{1\kappa}^0, j \in E_{2\kappa}^0, q \in K_{i\kappa}^0, r \in K_{j\kappa}^0, q = q_{ij}^{sp}$. Furthermore, a new vector $Z_\kappa^{\dot{\iota}}$ which includes new components of the set Z_{ij}^{spq} , $q \in B_{ij\kappa}^{sp} \cup C_{ij\kappa}^{sp}$, is formed. It is evident that $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*) \in \Theta_{\kappa+1}$. Thus, if at least one $k_{ij}^{spq} > 0$, then we obtain a new inequality system $F_{\kappa+1}(u, \tilde{h}, Z_{\kappa+1}) \geq 0$ specifying a set $\Lambda_{\kappa+1} \neq \Lambda_\kappa$ and a new starting point $\dot{\iota}$ where a new vector $Z_\kappa^{\dot{\iota}}$ includes components Z_{ij}^{spt} , $t \in B_{ij\kappa}^{sp} \cup C_{ij\kappa}^{sp}$. It follows from the construction that a starting point $(u^{\kappa*}, \tilde{h}^{\kappa*}, Z_\kappa^*)$ provides $H(\tilde{h}^{(\kappa+1)*}) \leq H(\tilde{h}^{\kappa*})$.

6.4. Computing a local minimum point on a feasible subregion

Since inequality system $F_\kappa(u, \tilde{h}, Z) \geq 0$ consists in general of a huge number of inequalities, the computation of local minimum point $(u^{\dot{\iota}}, \tilde{h}^{\dot{\iota}}, Z^{\dot{\iota}})$ of the problem

$$F(\tilde{\mathcal{H}}^{(\kappa+1)*}) = \min F(\tilde{\mathcal{H}}) \text{ s.t. } (u, \tilde{\mathcal{H}}, \mathbb{Z}) \in \Lambda_\kappa, \quad (7)$$

is also derived in stages.

Let a point $(u^{\kappa*}, \tilde{\mathcal{H}}^{\kappa*}, Z_\kappa^*) \in \Lambda_\kappa$ and some $\delta > 0$. Making use of spheres S_i with radii r_i^0 , $i \in I$, we select $\Psi_{ij}^{spt}(u_i, u_j, \mathbb{Z}_{ij}^{spt}) \geq 0$, $i \in A_{1\kappa}^t$, $j \in A_{2\kappa}^t$, $s \in K_i$, $p \in K_j$, $t = t_{ij}^{sp}$, from an inequality system $F_\kappa(v, \tilde{\mathcal{H}}, \mathbb{Z}_\kappa) \geq 0$ for which the inequalities $\|v_i^{\kappa*} - v_{i_j}^{\kappa*}\| - (r_i^0 + r_j^0) \leq \delta$, $i \in A_{1\kappa}^t$, $j \in A_{2\kappa}^t$, hold true.

Let $\mathbf{C} = \mathbf{C}_1$. In this case, we single out the inequalities $\Phi_{ik}^f(u_i, \tilde{\mathcal{H}}) \geq 0$, $i \in I_{f\kappa}$, $s \in K_i$, $f \in Y = \{1, 2, \dots, 6\}$, where $\Phi_{ik}^f(u_i, \tilde{\mathcal{H}})$ is a Φ -function for an object O_{is} and f -th half space, for which the inequalities

$$\begin{aligned} w_1 - x_i^{\kappa*} - r_i^0 &\leq \frac{\delta}{2}, i \in I_{1\kappa}, x_i^{\kappa*} + r_i^0 - w_2 \leq \frac{\delta}{2}, i \in I_{2\kappa}, \\ l_1 - y_i^{\kappa*} - r_i^0 &\leq \frac{\delta}{2}, i \in I_{3\kappa}, y_i^{\kappa*} + r_i^0 - l_2 \leq \frac{\delta}{2}, i \in I_{4\kappa}, \\ \eta_1 - z_i^{\kappa*} - r_i^0 &\leq \frac{\delta}{2}, i \in I_{5\kappa}, z_i^{\kappa*} + r_i^0 - \eta_2 \leq \frac{\delta}{2}, i \in I_{6\kappa} \end{aligned}$$

are fulfilled.

Next, we cover convex objects O_{ik} with spheres \mathbf{C}_{ik} of minimum radii ρ_{ik} and centers $v_{ik} = (x_{ik}, y_{ik}, z_{ik})$, $i \in I$, $k \in K_i$. We suppose that the origins of the local coordinate systems of O_{ik} coincide with the centers \mathbf{C}_{ik} , $i \in I$, $k \in K_i$. Then, the coordinates of centers of circles \mathbf{C}_{ik} with respect to the global coordinate systems of O_i are $v_{ik}(u_i) = (x_{ik}(u_i), y_{ik}(u_i), z_{ik}(u_i)) = R_i^T(v_{ik} + v_i)$, $i \in I$, $k \in K_i$.

Now let us choose inequalities $\Psi_{ij}^{spt}(u_i, u_j, \mathbb{Z}_{ij}^{spt}) \geq 0$, $i \in A_{1\kappa}^{0t} \subset A_{1\kappa}^t$, $j \in A_{2\kappa}^{0t} \subset A_{2\kappa}^t$, $s \in K_i^t \subset K_i$, $p \in K_j^t \subset K_j$, and $\Phi_{ik}^f(u_i, \tilde{\mathcal{H}}) \geq 0$, $i \in I_{f\kappa}$, $s \in K_{\kappa i}^f \subset K_i$, $f \in Y$, for which the inequalities

$$\begin{aligned} \|v_{is}(u_i^{\kappa*}) - v_{jp}(u_j^{\kappa*})\| - (\rho_{is} + \rho_{jp}) &\leq \delta, i \in A_{1\kappa}^{0t}, j \in A_{2\kappa}^{0t}, s \in K_i^t, p \in K_j^t, \\ w_1 - x_{ik}(u_i^{\kappa*}) - r_i^0 &\leq \frac{\delta}{2}, i \in I_{1\kappa}, k \in K_{\kappa i}^1, x_i(u_i^{\kappa*}) + r_i^0 - w_2 \leq \frac{\delta}{2}, i \in I_{2\kappa}, k \in K_{\kappa i}^2, \\ l_1 - y_i(u_i^{\kappa*}) - r_i^0 &\leq \frac{\delta}{2}, i \in I_{3\kappa}, k \in K_{\kappa i}^3, y_i(u_i^{\kappa*}) + r_i^0 - l_2 \leq \frac{\delta}{2}, i \in I_{4\kappa}, k \in K_{\kappa i}^4, \\ \eta_1 - x_i(u_i^{\kappa*}) - r_i^0 &\leq \frac{\delta}{2}, i \in I_{5\kappa}, k \in K_{\kappa i}^5, x_i(u_i^{\kappa*}) + r_i^0 - \eta_2 \leq \frac{\delta}{2}, i \in I_{6\kappa}, k \in K_{\kappa i}^6, \end{aligned}$$

are satisfied respectively.

Taking inequalities $\Psi_{ij}^{spt}(u_i, u_j, Z_{ij}) \geq 0$, $i \in A_{1\kappa}^{0t}$, $j \in A_{2\kappa}^{0t}$, $s \in K_i^t$, $p \in K_j^t$, $\Phi_{ik}^f(u_i, \tilde{\mathcal{H}}) \geq 0$, $i \in I_{f\kappa}$, $s \in K_{\kappa i}^f \subset K_i$, $f \in Y$, and $L(\tilde{\mathcal{H}}) \geq 0$, we form the inequality subsystem

$$F_{\kappa t}(u, \tilde{\mathcal{H}}, \mathbb{Z}_\kappa) = \begin{cases} \Psi_{ij}^{spt}(v_i, v_j, Z_{ij}) \geq 0, i \in A_{1\kappa}^{0t}, j \in A_{2\kappa}^{0t}, s \in K_i^t, p \in K_j^t, \\ \Phi_{ik}^f(u_i, \tilde{\mathcal{H}}) \geq 0, i \in I_{f\kappa}, s \in K_{\kappa i}^f \subset K_i, f \in Y, \\ L(\tilde{\mathcal{H}}) \geq 0, \\ \|v_{is}(u_i^{\kappa*}) - v_{st}(u_i)\| \leq \frac{\delta}{2}, i \in A_{1\kappa}^{0t}, s \in K_i^f \\ \|v_{is}(u_i^{\kappa*}) - v_{jp}(u_i)\| \leq \frac{\delta}{2}, j \in A_{2\kappa}^{0t}, p \in K_i^f, \end{cases} = \begin{cases} f_{i_1\kappa t}(\xi_{i_1}) \geq 0 \\ f_{i_2\kappa t}(\xi_{i_2}) \geq 0 \\ \dots\dots\dots \\ f_{i_q\kappa t}(\xi_{i_q}) \geq 0 \end{cases}.$$

which describes a subregion $\Lambda_{\kappa t}$ such that $X^\kappa \in (u^{\kappa*}, \tilde{\mathcal{H}}^{\kappa*}, Z_\kappa^*) \in \Lambda_{\kappa t} \subset \Lambda_\kappa$.

Consequently, searching for a local minimum point of the problem (1) – (2) can be reduced to solving a sequence of subproblems

$$F(\tilde{\kappa}^{\kappa(t+1)}) = \min F(\tilde{\kappa}) \text{ s.t. } (u, \tilde{\kappa}) \in \Lambda_{\kappa t}, t=0,1,2,\dots, \quad (8)$$

where a local minimum point $(u^{\kappa t}, \tilde{\kappa}^{\kappa t}, Z^{\kappa t})$ of the $(t-1)$ -th problem is taken as a starting point for the t -th problem, and the point $(u^{\kappa*}, \tilde{\kappa}^{\kappa*}, Z_{\kappa}^*)$ is taken as a starting point for $t=0$.

The problems are solved until $F(\tilde{\kappa}^{\kappa(t+1)}) = F(\tilde{\kappa}^{\kappa t})$ is met, and the point $(u^{\kappa*}, \tilde{\kappa}^{\kappa*}, Z_{\kappa}^*)$ is taken as a local minimum point of the problem (8).

We can diminish the problem dimension for each t . Considering a starting point $(u^{\kappa l}, \tilde{\kappa}^{\kappa l}, Z^{\kappa l})$ for the problem $F(\tilde{\kappa}^{\kappa(t+1)}) = \min F(\tilde{\kappa})$ s.t. $(v, \tilde{\kappa}) \in \Lambda_{\kappa t}$, we fix $Z^{\kappa t}$ (i.e., appropriate components of $Z^{\kappa t}$ do not vary). This means that $\Gamma_{\kappa t}(u, \tilde{\kappa}) = F_{\kappa t}(u, \tilde{\kappa}, Z^{\kappa t})$ and specifies the feasible subregion $\Lambda_{\kappa t}^z$ whose dimension is less than that of $\Lambda_{\kappa t}$. It is evident that $(u^{\kappa t}, \tilde{\kappa}^{\kappa t}) \in \Delta_{\kappa t}^z$ and all points of $\Delta_{\kappa t}^z$ ensure non-overlapping objects $O_i, i \in I$. Thus, we solve a sequence of problems $H(\tilde{\kappa}^{\kappa(t+1)}) = \min H(\tilde{\kappa})$ s.t. $(u, \tilde{\kappa}) \in \Delta_{\kappa t}^z, t=1,2,\dots$, until $H(\tilde{\kappa}^{\kappa(t+1)}) = H(\tilde{\kappa}^{\kappa t})$ is met. Obviously, the point $(u^{\kappa(t+1)}, \tilde{\kappa}^{\kappa(t+1)}, Z^{\kappa t})$ is not generally a local minimum point of the problem (8).

Taking the point $(u^{\kappa(t+1)}, \tilde{\kappa}^{\kappa(t+1)}, Z^{\kappa t})$ as a starting one, we continue to solve the problems (8) until a local minimum point $(u^{\kappa}, \tilde{\kappa}^{\kappa}, Z^{\kappa})$ of the problem (1) is obtained.

7. Computational modelling and numerical results

The efficacy of the proposed methodology is substantiated through the presentation of several case studies. The experiments were conducted on an Intel Core i5-750 computer, utilizing the IPOPT code for local optimization developed by [20].

IPOPT (Interior Point Optimiser) is a distinguished open-source solution for nonlinear optimization problems (NLPS), particularly when dealing with substantial datasets. The subsequent points highlight IPOPT's strengths, substantiated by insights gleaned from the given points:

1. Effective Performance with Large-Scale Challenges.

Utilization of Sparse Matrices: IPOPT employs sparse linear algebra techniques (MUMPS) to address extensive NLPS efficiently. This approach leads to a reduction in memory requirements and an acceleration in processing times.

Parallel linear solvers: The capacity to integrate with parallel solvers, such as HSL MA97 and MUMPS via MPI, provides the scalability necessary for high-dimensional problems.

Finally, IPOPT, an extension, reuses KKT matrix factorizations generated by IPOPT. This approach enables sensitivity calculations with minimal added computational expense, offering gains for parametric analysis and model predictive control.

2. A Reliable and Robust Algorithmic Approach

Interior-point methods: IPOPT utilizes a barrier method to address inequality constraints by incorporating logarithmic penalties. This ensures stability even when confronting degenerate scenarios.

Hybrid optimization methods: IPOPT employs an intelligent blend of gradient-based optimizers, such as the quasi-Newton L-BFGS, with exact Hessian information to achieve accelerated convergence.

Finally, the paper discusses penalty methods. Implementing penalty methods enhances the robustness of the approach when confronted with degenerate nonlinear programming (NLP) problems. This technique meticulously balances feasibility and optimality, yielding superior outcomes compared to standard barrier methodologies in complex scenarios.

3. The flexibility in problem formulation constitutes a significant advantage of IPOPT.

Mathematical Programming with Equilibrium Constraints (MPCC): A notable feature of IPOPT is its ability to circumvent the need for mixed-integer formulations when dealing with non-smooth problems, such as those involving absolute values. This property of IPOPT serves to streamline the implementation process.

Constraint satisfaction: IPOPT can address nonlinear systems by rephrasing them as nonlinear programs (NLPS) that utilize a trivial objective function (e.g., maximizing 0 subject to $f(x) = 0$).

4. Integration with Contemporary Tools.

Open-source ecosystem: IPOPT offers seamless interoperability with platforms like Julia, Python, and MATLAB, which enables antidifferentiation capabilities alongside facilitating higher-level modelling approaches.

IPOPT's forte lies in the domain of solving large, sparse NLPs. This is primarily attributable to its advanced interior-point framework, efficient sparse linear algebra integration, and adaptability in addressing many problem types. Furthermore, its open-source foundation and ease of use with modern tools make IPOPT indispensable for chemical engineering, economics, and applications in real-time control systems. Optimized outcomes are achieved by pairing it with high-performance linear solvers, such as HSL MA57, and extensions like IPOPT to facilitate effective sensitivity analysis.

The algorithm was tested on various benchmark instances from [14], with the results summarized below.

For packing 36 objects (Fig. 1a): the HAPE3D approach yielded a volume of 12.4 and a runtime of 963 seconds, while our method attained a volume of 10.7 and a runtime of 750 seconds.

For the case of packing 40 objects (Fig. 1b): the HAPE3D approach achieved a volume of 61.9 and a runtime of 999 seconds, while our method achieved a volume of 56.0 and a runtime of 533 seconds. The results of this study are illustrated in Figure 1.

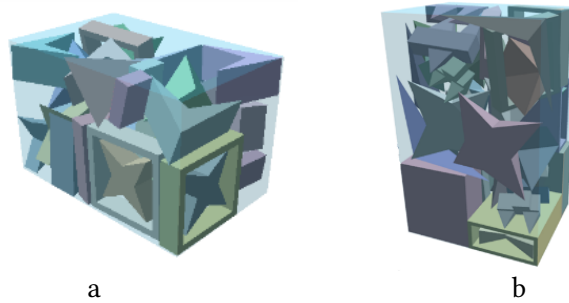


Figure 1: Comparison of the results obtained with the results presented in [14]: a) 36 non-convex polyhedra; b) 40 non-convex polyhedra.

As demonstrated in Figure 2, the intelligent system developed for this study successfully packed 300 non-convex polyhedra. This result demonstrates the system's capacity to address high-dimensional problems while effectively maintaining adequate time performance.

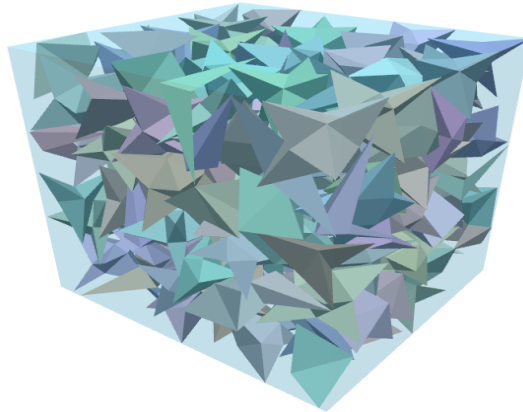


Figure 2: Result of packing of 300 objects

The effectiveness of the proposed approach is confirmed by comparing the results of packing non-convex polyhedra with the results presented by the paper's authors [14]. The results of this comparison are shown in Figure 3.

The results demonstrate that the proposed Intelligent Geometric Modeling Framework significantly reduces computation time and enhances the performance metrics across the test cases.

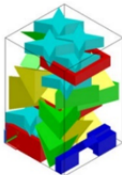
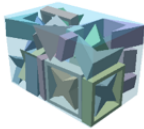
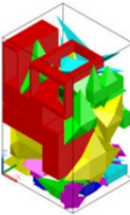
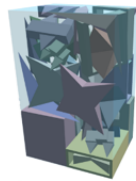
	<i>HAPE3D</i>	<i>Proposed approach</i>
The result of packing 36 objects		
Volume	12 480	10 720
Runtime (seconds)	9 637	4 789
Result illustration		
The result of packing 40 objects		
Volume	61 950	56 012
Runtime (seconds)	99 952	24 543
Result illustration		

Figure 3: Comparison of results

8. Conclusions

This article outlines a process for developing an intelligent system focused on geometric design. The proposed systems will leverage cutting-edge methods and tools to automate and improve how geometric shapes are arranged within a three-dimensional environment. The core benefit of these technologies will be their ability to find the best possible solutions when applied to practical challenges in additive manufacturing. Artificial intelligence and other novel techniques will be central to achieving optimal results with these systems.

This research introduces a novel method for precisely modelling the three-dimensional irregular packing problem. Employing the phi-function method, we can leverage contemporary nonlinear optimization techniques to address this challenge, including creating initial configurations and determining local minima.

The clustering technique facilitates starting point generation by solving the packing problem involving half the quantity of convex objects characterized by simpler shapes. This strategic simplification notably diminishes the computational requirements of establishing the initial configurations.

The procedure's computational performance is improved by employing a two-step strategy to locate the local optimum. Initially, a linear problem is addressed. A nonlinear problem then succeeds this in the subsequent stage. The displayed results clearly demonstrate the efficacy of this method in finding solutions for the particular irregular packing problem being studied.

This approach significantly improves the accuracy and efficiency of solving 3D packing issues, which has vital implications for the progress of both natural and information systems. This combination exemplifies a strong synergy between mathematical modelling and advanced computational tools. The approach enhances the precision and efficiency of 3D packing solutions, essential for advancing natural and information systems. This integration demonstrates the powerful collaboration between mathematical models and computational techniques.

Declaration on Generative AI

During the preparation of this work, the authors used Grammarly in order to: Grammar and spelling check. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the publication's content.

References

- [1] X. Cui, X. Li, Y. Du, X. Zhang, J. Hao, Y. Hu, Macro-micro numerical analysis of granular materials considering principal stress rotation based on DEM simulation of dynamic hollow cylinder test, *Construction and Building Materials* 412 (2024) 134818, doi:10.1016/j.conbuildmat.2023.134818.
- [2] S. Guan, T. Qu, Y. T. Feng et al. A machine learning-based multi-scale computational framework for granular materials, *Acta Geotech.* 18 (2023) 1699–1720. doi:10.1007/s11440-022-01709-z.
- [3] H. Zhao, Z. Pan, Y. Yu, K. Xu, Learning Physically Realizable Skills for Online Packing of General 3D Shapes, *ACM Trans. Graph.* 42 (5) (2023). doi:10.1145/3603544.
- [4] B. Guo, Y. Zhang, J. Hu, J. Li, F. Wu, Q. Peng, Q. Zhang, Two-dimensional irregular packing problems: A review, *Front. Mech. Eng* 8 (2022) 1–15. doi:10.3389/fmech.2022.966691.
- [5] T. Romanova, Yu. Stoyan, A. Pankratov, et al., Optimized packing soft ellipses, in: *Human-Assisted Intelligent Computing*, IOP Publishing, 2023, pp. 9.1–9.16. doi:10.1088/978-0-7503-4801-0ch9.
- [6] B. Zhang, Y. Yao, H. K. Kan et al, A GAN-based genetic algorithm for solving the 3D bin packing problem, *Sci Rep* 14 (2024). doi:10.1038/s41598-024-56699-7.
- [7] A. Pankratov, T. Romanova, I. Litvinchev, Packing Oblique 3D Objects. *Mathematics* 8(7) (2020). doi:10.3390/math8071130.
- [8] Z. Wang, Y. Wu, An Ant Colony Optimization-Simulated Annealing Algorithm for Solving a Multitask AGVs Workshop Scheduling Problem with Limited Buffer Capacity, *Processes* 11 (2023). doi:10.3390/pr11030861.
- [9] J. Kallrath, Cutting and Packing Beyond and Within Mathematical Programming, in: *Business Optimization Using Mathematical Programming*, International Series in Operations Research & Management Science, vol 307, Springer, Cham, 2021, pp. 495–526. doi:10.1007/978-3-030-73237-0_15.
- [10] Y. Ma, Z. Chen, W. Hu, W. Wang, Packing Irregular Objects in 3D Space via Hybrid Optimization. *Computer Graphics Forum* 37(8) (2018) 134–150. doi:10.1111/cgf.13490.
- [11] T.-H. Nguyen, X.-T. Nguyen, Space Splitting and Merging Technique for Online 3-D Bin Packing, *Mathematics* 11 (2023). doi:10.3390/math11081912.
- [12] A. Kurpisz, A. Suter, Improved Approximations for Translational Packing of Convex Polygons, *arXiv:2308.08523* (2023). doi:10.48550/arXiv.2308.08523.
- [13] C. Lamas-Fernandez, J. A. Bennell, A. Martinez-Sykora, Voxel-based solution approaches to the three-dimensional irregular packing problem, *Operations Research* 71(4) (2023) 1298–1317. doi:10.1287/opre.2022.2260.
- [14] X. Liu, J. Liu, A. Cao, Z. Yao, HAPE3D – a new constructive algorithm for the 3D irregular packing problem, *Frontiers of Information Technology & Electronic Engineering* 16(5) (2015) 380–390. doi:10.1631/FITEE.1400421.
- [15] Y.K. Joung, S. D. Noh, Intelligent 3D packing using a grouping algorithm for automotive container engineering, *Journal of Computational Design and Engineering* 1(2) (2014) 140–151. doi:10.7315/JCDE.2014.014.
- [16] J. Kallrath, Packing ellipsoids into volume-minimizing rectangular boxes, *Journal of Global Optimization* 67(1-2) (2017) 151–185. doi:10.1007/s10898-015-0348-6.
- [17] G. Yaskov, A. Chugay, Packing Equal Spheres by Means of the Block Coordinate Descent Method, *CEUR Workshop Proceedings* 2608 (2020) 150–160. doi:10.32782/cm15/2608-13.
- [18] Y. E. Stoian, A. M. Chugay, A. V. Pankratov et al, Two Approaches to Modeling and Solving the Packing Problem for Convex Polytopes, *Cybern Syst Anal* 54 (2018) 585–593, doi:10.1007/s10559-018-0059-3.
- [19] A. M. Chugay, A. V. Zhuravka, Packing Optimization Problems and Their Application in 3D Printing, in: Z. Hu, S. Petoukhov, I. Dychka, M. He (eds.), *Advances in Computer Science for Engineering and Education III. ICCSEE 2020*, Advances in Intelligent Systems and Computing, vol 1247, Springer, Cham, 2021, pp. 75–85. doi:10.1007/978-3-030-55506-1_7.
- [20] A. Wächter, L. Biegler, On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming, *Math. Program.* 106 (2006) 25–57. doi:10.1007/s10107-004-0559-y.